Solving the time-dependent Schrödinger Eq.

$$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi$$

$$\frac{\partial}{\partial t}\psi = \frac{1}{i\hbar}\underbrace{\Big(\overbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}^{=T} + \overbrace{V(x)}^{=V}\Big)}\psi$$

$$\int \underbrace{\frac{1}{\psi}\frac{\partial \psi}{\partial t}} = \int \frac{1}{i\hbar}(T+V)\,dt \quad \text{no explicit time-dep.}$$

$$\int \underbrace{\frac{\partial}{\partial t}\ln\psi}_{''\ln\psi} = +\frac{1}{i\hbar}t(T+V) + C$$

$$\Rightarrow \quad \psi = e^{+\frac{1}{i\hbar}t(T+V)}e^{C}$$

$$\boxed{\psi(t) = e^{-\frac{it}{\hbar}(T+V)}\psi(0)}$$

For the case $V=0$, free propagation

Take $\psi(x,0) = e^{ikx}$

$$\psi(t) = e^{-i\frac{t}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)}e^{ikx}$$

$$= e^{\alpha\frac{\partial^2}{\partial x^2}}e^{ikx} \qquad \alpha = \frac{it}{\hbar}\frac{\hbar^2}{2m}$$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\alpha^n\left(\frac{\partial^2}{\partial x^2}\right)^n e^{ikx} \qquad \uparrow$$

$$\frac{\partial^2}{\partial x^2}e^{ikx} = (-k^2)e^{ikx}$$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\alpha^n(-k^2)^n e^{ikx}$$

$$= e^{\alpha(-k^2)}e^{ikx}$$

$$\boxed{\psi(x,t) = e^{-\frac{i}{\hbar}t\frac{\hbar^2}{2m}k^2}e^{ikx} = (\psi(x,0))}$$ exact propagation of a plane wave

Therefore in general

$$\psi(x,0) = \int dk\, e^{ikx}\psi(k,0)$$ ↖ Fourier transform

$$\psi(x,t) = e^{-i\frac{t}{\hbar}T}\psi(x,0)$$

$$= \int dk\, e^{-\frac{i}{\hbar}t\frac{\hbar^2}{2m}k^2}e^{ikx}\psi(k,0)$$

$$\psi(x,t) = \int dk\, e^{ikx}\left[e^{-\frac{i}{\hbar}t\frac{\hbar^2}{2m}k^2}\psi(k,0)\right]$$

$$\uparrow$$

$$\psi(k,0) = \text{FT of } \psi(x,0)$$

$$= \frac{1}{2\pi}\int dx'\, e^{-ikx'}\psi(x',0) \quad \Leftarrow$$ takes N^2 operations

$$\psi(x,0) = \int dk\, e^{ikx}\psi(k,0)$$

$$= \frac{1}{2\pi}\int dx' \underbrace{\int dk\, e^{ik(x-x')}}_{2\pi\,\delta(x-x')}\psi(x',0)$$

$$= \psi(x,0)$$

Given $\psi(x,0)$, take the FFT $\sim N \ln N$ operations

$x_i = i\Delta x$ i.e. $\psi(x_i, 0)$ fast

$(M)(V) \Rightarrow N^2 \Rightarrow N \ln N$

$N \sim 10^3$

$N^2 \sim 10^6$ $N \ln N \propto 10^3$

to produce the momentum-space wf

$FFT(\psi(x,0)) = \psi(k,0) = \psi(k_i, 0)$ $k_i = i\Delta k$

The kinetic energy propagation is the just

$$e^{-\frac{i}{\hbar}t\left(\frac{\hbar^2 k_i^2}{2m}\right)}\psi(k_i,0) = \tilde{\psi}(k,0)$$

finally backward FFT to $\psi(x,t)$

$$\psi(x,t) = FFT^{-1}(\tilde{\psi}(k,0))$$

$$= FFT^{-1}\left(e^{-\frac{i}{\hbar}t\left(\frac{\hbar^2 k^2}{2m}\right)} FFT(\psi(x,0))\right)$$

For a position-based wf $\psi(x,0)$, then the pot. operator is just a pt-by-pt multiplication

$$\psi(x,t) = e^{-i\frac{t}{\hbar}V(x)}\psi(x,0)$$

Since the propagation of T & V can be "exactly" computed, therefore

$$\psi(t+\Delta t) = \underbrace{e^{-i\frac{\Delta t}{\hbar}(T+V)}}_{\text{factorize or split the evolution op.}}\psi(t)$$

1st order $\sim e^{-i\frac{\Delta t}{\hbar}T}\, e^{-i\frac{\Delta t}{\hbar}V}\,\psi(t)$

2nd order $\underbrace{e^{-\frac{i}{\hbar}(\frac{1}{2}\Delta t)V}}_{\text{pt-pt multiplication}}\ \underbrace{e^{-i\frac{\Delta t}{\hbar}T}}_{FFT \times e^{-\frac{i}{\hbar}\Delta t\left(\frac{\hbar^2 k^2}{2m}\right)}\ FFT^{-1}}\ \underbrace{e^{-\frac{i}{\hbar}(\frac{1}{2}\Delta t)V}}_{\text{pt-pt multiplication}}\ \psi(x,t)$

any higher order factorization of $e^{t(T+V)}$ will give rise to an alg. for solving the S.Eq.

Generalize easily to 3D by taking 3D FFT.

$$\psi(x,y,z) \to \psi(i\Delta x, j\Delta y, k\Delta z)$$

complex

$n_x\, n_y\, n_z \to 10^6$

$10^2\ 10^2\ 10^2$

i.e. 2 particle $\sim 10^{12}$

3 — 10^{18}

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